

Patrick K. Schelling
Curriculum Vitae

Professional Preparation

University of Minnesota, Minneapolis, MN	Ph.D. 1999	Physics
University of Minnesota, Minneapolis, MN	B.S. 1992	Physics

Appointments

5/09-present Associate Professor, Department of Physics, U. of Central Florida, Orlando, FL
8/03-5/09: Assistant Professor, Department of Physics, U. of Central Florida, Orlando, FL
5/01-7/03: Visiting Scientist, Materials Science Division, Argonne National Laboratory, Argonne IL and Institute for Nanotechnology, Karlsruhe Germany
8/99-5/01: Postdoctoral Researcher, Materials Science Division, Argonne National Laboratory, Argonne IL (advisers Simon Phillpot, Dieter Wolf)
8/95-8/99: Graduate Research Assistant, Physics Department, University of Minnesota, Minneapolis MN (adviser J. Woods Halley)

Refereed Journal Articles:

1. B. Doan, A. R. Dove, and P. K. Schelling, "Dissipation and adhesion between amorphous FeO nanoparticles," *J. Aero. Sci.* **in press** (2021)
2. K. Barmak, S. Ezzat, R. Gusley, A. Jog, S. Kerdsongpanya, A. Khanya, E. Milosevic, W. Richardson, K. Sentosun, A. Zangiabadi, D. Gall, W. E. Kaden, E. R. Mucciolo, P. K. Schelling, A. C. West, and K. R. Coffey, "Epitaxial metals for interconnects beyond Cu", *J. Vac. Sci. Tech. A* **38**, 033406 (2020)
3. K. Fernando and P. K. Schelling, "Non-local linear-response functions for thermal transport computed with equilibrium molecular-dynamics simulation," *J. Appl. Phys.* **128**, 215105 (2020)
4. W. C. Tucker, A. R. Dove, and P. K. Schelling, "Dissipation and plastic deformation in collisions between metallic nanoparticles," *Comp. Mat. Sci.* **161**, 214-222 (2019)
5. A. H. Quadery, B. Doan, W. C. Tucker, A. Dove, and P. K. Schelling, "Role of surface chemistry in grain adhesion and dissipation during collisions of silica nanograins," *The Astrophysical Journal* **84**, 105 (2017)
6. W. C. Tucker, A. H. Quadery, P. K. Schelling, A. Schulte, R. Blair, W. Kaden, and D. Britt, "Strong catalytic activity of iron nanoparticles on the surfaces of reduced olivine," *Icarus* **299**, 502-512 (2018)
7. W. C. Tucker and P. K. Schelling, "Thermodiffusion in liquid binary alloys computed from molecular-dynamics simulation and the Green-Kubo formalism," *Comp. Mat. Sci.* **124**, 54-61 (2016)
8. Abrar Quadery, Shaun Pacheco, Alan Au, Natalie Rizzacasa, Joshua Nichols, Timothy Le, Cameron Glasscock, and Patrick K. Schelling, "Atomic-scale simulation of radiation damage in olivine and orthopyroxene," *J. Geophys. Res. Planets* **120**, 643-661 (2015)

9. W. C. Tucker and P. K. Schelling, "Analysis of simulation methodology for calculation of the heat of transport for vacancy thermodiffusion," *J. Appl. Phys.* **116**, 023504 (2014)
10. P. K. Schelling, J. Ernotte, W. C. Tucker, J. W. Halley, and L. Shokeen, "Molecular-dynamics calculation of the vacancy heat of transport," *J. Appl. Phys.* **116**, 023506 (2014)
11. D. Choi, X. Liu, P. K. Schelling, K. R. Coffey, and K. Barmak, "Failure of Theoretical Models to Describe Resistivity of Nanometric, Polycrystalline Tungsten Films," *J. Appl. Physics*, **115**, 104308 (2014)
12. W. Tucker, L. Shokeen, and P. K. Schelling, "Atomic-scale simulation of the thermodiffusion of hydrogen in palladium," *J. Appl. Phys.* **114**, 063509 (2013)
13. M. Sheng, P. K. Schelling, and P. Keblinski, "Heat transfer mechanism across few-layer graphene by molecular dynamics", *Phys. Rev. B.* **88**, 045444 (2013)
14. L. Shokeen and P. K. Schelling, "Role of electronic-excitation effects in the melting and ablation of laser-excited silicon," *Comp. Mat. Sci.* **67**, 316 (2013)
15. P. K. Schelling and T. Le, "Computational methodology for analysis of the Soret effect in crystals: Application to hydrogen in palladium," *J. Appl. Phys.* **112**, 083516 (2012)
16. Y. Chen, A. Chernatynskiy, D. Brown, P. K. Schelling, E. Artacho, and S. R. Phillpot, "Critical assessment of classical potentials for MgSiO₃ perovskite with application to thermal conductivity calculations," *Phys. Earth Plan. Inter.* **210-211**, 75 (2012)
17. Z. McDargh and P. K. Schelling, "Molecular-dynamics approach for determining the vacancy heat of transport," *Comp. Mat. Sci.* **50**, 2363 (2011)
18. L. Shokeen and P. K. Schelling, "Thermodynamics and kinetics of silicon under conditions of strong electronic excitation," *J. Appl. Phys.* **109**, 073503 (2011)
19. L. Shokeen and P. K. Schelling, "An empirical potential for silicon under conditions of strong electronic excitation," *Appl. Phys. Lett.* **97**, 151907 (2010)
20. P.K. Schelling, "Thermal conductivity of A-site doped pyrochlore oxides studied by molecular-dynamics simulation," *Comp. Mat. Sci.* **48**, 336 (2010)
21. T. Watanabe, S.G. Srivilliputhur, P.K. Schelling, J.S. Tulenko, S.B. Sinnott, and S.R. Phillpot, "Thermal Transport in Off-stoichiometric Uranium Dioxide by Atomic Level Simulation," *J. Am. Ceram. Soc.* **92**, 850 (2009)
22. Ming Hu, P. Keblinski, and P.K. Schelling, "Kapitza conductance of silicon-amorphous polyethylene interfaces by molecular-dynamics simulation," *Phys. Rev. B* **79**, 104305 (2009)
23. X.W. Zhou, S. Aubry, R.E. Jones, A. Greenstein, and P.K. Schelling, "Towards More Accurate Molecular Dynamics Calculations of Thermal Conductivity. Case study: GaN Bulk Crystals," *Phys. Rev. B* **79**, 115201 (2009)
24. S. Aubry, C. Kimmer, A. Skye, and P.K. Schelling, "Comparison of theoretical and simulation-based predictions of grain-boundary Kapitza conductance in silicon," *Phys. Rev. B* **78**, 064112 (2008)
25. P.K. Schelling, "Phase diagram and kinetics of a new bond-order potential for silicon," *Comp. Mat. Sci.* **44**, 274 (2008)
26. T. Watanabe, S.B. Sinnott, J.S. Tulenko, R.W. Grimes, P.K. Schelling, and S.R. Phillpot, "Thermal Transport Properties of Uranium Dioxide by Molecular Dynamics Simulation," *J. Nucl. Mat.* **375**, 388 (2008)